

# Two Gaussian Approaches to Black-Box Optimization

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## 1 CMA Evolution Strategy

*CMA-ES* [7, 8] is the state-of-the-art evolutionary optimization method, at least in the area of continuous black-box optimization. Basically, it consists in generating new search points by sampling from a multidimensional normal distribution, the mean and variance of which are updated from generation to generation. In particular, the population  $x_1^{(g+1)}, \dots, x_\lambda^{(g+1)} \in \mathbb{R}^d$  of the  $g + 1$ -st generation,  $g \geq 1$ , follows the normal distribution with mean  $m^{(g)} \in \mathbb{R}^d$  and variance  $(\sigma^{(g)})^2 C^{(g)} \in \mathbb{R}^{d,d}$  resulting from the update in the  $g$ -th generation,

$$x_i^{(g+1)} \sim N(m^{(g)}, (\sigma^{(g)})^2 C^{(g)}). \quad (1)$$

Here,  $\sigma^{(g)}$  is the step size in the  $g$ -th generation.  $C^{(g)} \in \mathbb{R}^{d,d}$  and  $\sigma^{(g)} > 0$  are updated separately,  $C^{(g)}$  being in the most simple case obtained as the unbiased empirical estimate based on the  $g$ -th generation:

$$C_{\text{emp}}^{(g)} = \frac{1}{\lambda - 1} \sum_{i=1}^{\lambda} \left( x_i^{(g)} - \frac{1}{\lambda} \sum_{j=1}^{\lambda} x_j^{(g)} \right) \left( x_i^{(g)} - \frac{1}{\lambda} \sum_{j=1}^{\lambda} x_j^{(g)} \right)^{\top}. \quad (2)$$

The positive semidefinite matrix  $C^{(g)}$  can be diagonalised in the basis formed by its eigenvectors  $b_1^{(g)}, \dots, b_d^{(g)}$ ,

$$C^{(g)} = B^{(g)} D^{(g)} B^{(g)\top}, \quad (3)$$

where  $B^{(g)} = (b_1^{(g)} \dots b_d^{(g)})$  and  $D^{(g)}$  is a diagonal matrix such that its  $k$ -th diagonal element is the eigenvalue corresponding to the eigenvector  $b_k^{(g)}$ . Consequently, the coordinates of points generated according to (1) in that basis,  $\{x_i^{(g+1)}\}^{B^{(g)}}$ , are uncorrelated:

$$\{x_i^{(g+1)}\}^{B^{(g)}} = B^{(g)\top} x_i^{(g+1)} \sim N(B^{(g)\top} m^{(g)}, (\sigma^{(g)})^2 B^{(g)\top} C^{(g)} B^{(g)}). \quad (4)$$

## 2 Optimization Based on Gaussian Processes

A *Gaussian process (GP)* on a  $d$ -dimensional Euclidean space  $\mathbb{X}$  is a collection of random variables,  $\text{GP}_{\mathbb{X}} = (f(x))_{x \in \mathbb{X}}$ , such that the joint distribution of any finite number of them is a multidimensional normal distribution. Following [4], we differentiate two ways of using GPs in black-box optimization:

- (i) As a *surrogate model* to be optimized instead of the black box objective function. On the found optimum or optima, the original black-box objective function is then evaluated. This use of GPs has been introduced in the popular Efficient Global Optimization (EGO) algorithm [14]. As the optimization method, also evolutionary optimization can be used, in particular CMA-ES [4], but this is not the only possibility: For example, traditional low-degree polynomial models, aka response surface models [20], are much more efficiently optimized using traditional smooth optimization methods.
- (ii) For the *evolution control* of the evolutionary optimization of the original objective function, i.e., for controlling the composition of its population [5, 6, 9, 23].

Irrespective of the way in which a GP is used, its construction is always based on a sequence  $(x_1, y_1), \dots, (x_n, y_n) \in \mathbb{X} \times \mathbb{R}$  of training pairs and is subsequently employed to compute the random variable  $f(x)$  for  $x \notin \{x_1, \dots, x_n\}$ . Since the distribution of  $(f(x), f(x_1), \dots, f(x_n))$  is multidimensional normal, also the conditional distribution of  $f(x)$  conditioned on  $f(x_1), \dots, f(x_n)$  is normal,

$$f(x)|f(x_1), \dots, f(x_n) \sim N(\mu(x; X, Y), \Sigma(x; X, Y)), \quad (5)$$

where  $X = (x_1, \dots, x_n), Y = (y_1, \dots, y_n), \mu(\cdot; X, Y) : \mathbb{X} \rightarrow \mathbb{R}, \Sigma(\cdot; X, Y) : \mathbb{X} \rightarrow \mathbb{R}^2$ . There are two commonly encountered possibilities how define the functions  $\mu(\cdot; X, Y)$ , describing the conditional GP mean, and  $\Sigma(\cdot; X, Y)$ , describing the conditional GP variance:

1. A GP is the *superposition of a deterministic function*  $\bar{f} : \mathbb{X} \rightarrow \mathbb{R}$  and a GP with zero mean. For the latter, it can be shown [21] that the function describing its mean fulfils

$$(\forall x \in \mathbb{X}) \mu_0(x; X, Y) = K(x, X)(K(X, X) + \sigma_{\text{noise}}^2 I_n)^{-1} Y^\top, \quad (6)$$

whereas the function describing its variance fulfills

$$(\forall x \in \mathbb{X}) \Sigma_0(x; X, Y) = K(x, x) - K(x, X)(K(X, X) + \sigma_{\text{noise}}^2 I_n)^{-1} K(X, x). \quad (7)$$

Here, an i.i.d. Gaussian noise is assumed,  $I_n$  is the  $n$ -dimensional identity matrix,  $K : \mathbb{X} \times \mathbb{X} \rightarrow \mathbb{R}$  is a symmetric function, and

$$\begin{aligned} K(x, X) &= (K(x, x_1), \dots, K(x, x_n)), K(X, x) = K(x, X)^\top, \\ K(X, X) &= (K(x_1, X)^\top, \dots, K(x_n, X)^\top)^\top. \end{aligned} \quad (8)$$

The resulting superposition then fulfils

$$(\forall x \in \mathbb{X}) \mu(x; X, Y) = \bar{f}(x) + K(x, X)(K(X, X) + \sigma_{\text{noise}}^2 I_n)^{-1} (Y - (\bar{f}(x_1), \dots, \bar{f}(x_n)))^\top, \quad (9)$$

whereas  $\Sigma = \Sigma_0$ .

2. A GP is the *superposition of a Bayesian mean assuming the multiplicative form*  $w\bar{f}$  and a GP with zero mean, where  $w$  is a random variable with  $w \sim N(1, \sigma_w^2), \sigma_w > 0$ ,

and  $\bar{f}$  has the same meaning as above. In that case, it can be shown [21] that for  $x \in \mathbb{X}$ ,

$$\mu(x; X, Y) = K(x, X)(K(X, X) + \sigma_{\text{noise}}^2 I_n)^{-1} Y^\top + (\bar{f}(x) - (\bar{f}(x_1), \dots, \bar{f}(x_n))(K(X, X) + \sigma_{\text{noise}}^2 I_n)^{-1} K(X, x)) \hat{w}, \quad (10)$$

$$\Sigma(x; X, Y) = K(x, x) - K(x, X)(K(X, X) + \sigma_{\text{noise}}^2 I_n)^{-1} K(X, x) + \frac{\sigma_w^2 (K(X, X) + \sigma_{\text{noise}}^2 I_n)^{-1} Y^\top + \hat{\kappa}^2}{1 + \sigma_w^2 (\bar{f}(x_1), \dots, \bar{f}(x_n))(K(X, X) + \sigma_{\text{noise}}^2 I_n)^{-1} (\bar{f}(x_1), \dots, \bar{f}(x_n))^\top}, \quad (11)$$

where

$$\hat{w} = \frac{1 + \sigma_w^2 (\bar{f}(x_1), \dots, \bar{f}(x_n))(K(X, X) + \sigma_{\text{noise}}^2 I_n)^{-1} (\bar{f}(x_1), \dots, \bar{f}(x_n))^\top}{1 + \sigma_w^2 (\bar{f}(x_1), \dots, \bar{f}(x_n))(K(X, X) + \sigma_{\text{noise}}^2 I_n)^{-1} Y^\top}, \quad (12)$$

$$\hat{\kappa} = (\bar{f}(x) - (\bar{f}(x_1), \dots, \bar{f}(x_n))(K(X, X) + \sigma_{\text{noise}}^2 I_n)^{-1} K(X, x)) \quad (13)$$

Simple, but frequently used examples of the function  $K$  occurring in (6)–(7) and (10)–(11) include:

- *Squared exponential*,

$$(\forall x, x' \in \mathbb{X}) \ K(x, x') = e^{-\frac{\|x-x'\|^2}{2\ell^2}}, \ell > 0. \quad (14)$$

Here,  $\ell$  is a parameter called *characteristic length-scale*. It is a parameter of the function  $K_{\text{SE}}$ , not of the Gaussian process, the process is nonparametric. Therefore  $\ell$  is referred to as a *hyperparameter*.

- *$\gamma$ -Exponential*,

$$(\forall x, x' \in \mathbb{X}) \ K(x, x') = e^{-\left(\frac{\|x-x'\|}{\ell}\right)^\gamma}, \ell > 0, 0 < \gamma \leq 2, \quad (15)$$

which has 2 hyperparameters,  $\lambda$  and  $\gamma$ .

- *Dot product*,

$$(\forall x, x' \in \mathbb{X}) \ K(x, x') = (\sigma^2 + x^\top x')^p, \sigma \geq 0, p \in \mathbb{N}, \quad (16)$$

which has 2 hyperparameters,  $\sigma$  and  $p$ , or in its generalized version,

$$(\forall x, x' \in \mathbb{X}) \ K(x, x') = (\sigma^2 + x^\top \Sigma x')^p, \Sigma \in \mathbb{R}^{d,d} \text{ positive definite}, \quad (17)$$

which has, in addition, the matrix of hyperparameters  $\Sigma$ , defining a dot product in general coordinates.

## 2.1 GP-based criteria to choose the points for evaluation

Whereas traditional response surface and surrogate models employ basically only one criterion for the choice of points in which the black box objective function should be evaluated, namely the global or at least local minimum of the model (if the optimization objective is minimization), GPs offer several additional criteria:

- (i) *Minimum of a prescribed quantile* ( $Q_\alpha$ ) of the distribution of  $f(x)|f(x_1), \dots, f(x_n)$ ,  $\alpha \in (0, 1)$ .

$$x_\alpha^* = \arg \min_{x \in \mathbb{X}} q_\alpha(N(\mu(x; X, Y), \Sigma(x; X, Y))). \quad (18)$$

Usually, (18) is expressed using quantiles of the standard normal distribution,  $u_\alpha = q_\alpha(N(0, 1))$ ,

$$x_\alpha^* = \arg \min_{x \in \mathbb{X}} \mu(x; X, Y) + \sqrt{\Sigma(x; X, Y)} u_\alpha = \arg \min_{x \in \mathbb{X}} \mu(x; X, Y) - \sqrt{\Sigma(x; X, Y)} u_{1-\alpha}. \quad (19)$$

For  $\alpha = 0.5$ , (19) turns to the traditional global minimum criterion, applied to  $\mu(\cdot; X, Y)$ .

- (ii) *Probability of improvement* ( $PoI$ ),

$$x_{PI}^* = \arg \max_{x \in \mathbb{X}} P(f(x) < f_{\min} | f(x_1), \dots, f(x_n)) = \phi \left( \frac{f_{\min} - \mu(x; X, Y)}{\sqrt{\Sigma(x; X, Y)}} \right), \quad (20)$$

where  $\phi$  denotes the distribution function of  $N(0, 1)$ ,  $f_{\min}$  is the minimum value found so far. More generally, *probability of improvement with respect to a given*  $T \leq f_{\min}$ ,

$$x_{PI-T}^* = \arg \max_{x \in \mathbb{X}} P(f(x) < T | f(x_1), \dots, f(x_n)) = \phi \left( \frac{T - \mu(x; X, Y)}{\sqrt{\Sigma(x; X, Y)}} \right). \quad (21)$$

- (iii) *Expected improvement* ( $EI$ ),

$$x_{EI}^* = \arg \max_{x \in \mathbb{X}} E((f_{\min} - f(x))I(f(x) < f_{\min}) | f(x_1), \dots, f(x_n)),$$

$$\text{where } I(f(x) < f_{\min}) = \begin{cases} 1 & f(x) < f_{\min}, \\ 0 & f(x) \geq f_{\min}. \end{cases} \quad (22)$$

Introducing the normalized mean improvement  $\nu : \mathbb{X} \rightarrow \mathbb{R}$ ,

$$(\forall x \in \mathbb{X}) \nu(x) = \frac{f_{\min} - \mu(x; X, Y)}{\sqrt{\Sigma(x; X, Y)}}, \quad (23)$$

and the notation  $\varphi$  for the density of  $N(0, 1)$ , (22) can be expressed as [13]

$$x_{EI}^* = \arg \max_{x \in \mathbb{X}} \sqrt{\Sigma(x; X, Y)} (\nu(x) \phi(\nu(x)) + \varphi(\nu(x))). \quad (24)$$

### 3 Possible Synergy

Directly connecting both considered Gaussian approaches is not possible because the normal distribution in CMA-ES is a distribution on the input space of the objective function (fitness), whereas the normal distribution in GPs is on the space of its function values. Nevertheless, it is still possible to achieve some synergy through using information from CMA-ES for the GP, and/or using information from the GP for CMA-ES. According to what was recalled at the beginning of Section 2, the latter possibility corresponds to using GP for the evolution control of CMA-ES.

#### 3.1 Using Information from CMA-ES for the GP

We see 2 straightforward possibilities where some information from CMA-ES can be used in the GP.

1. The function  $\bar{f}$  occurring in (9), (10) and (11) can be constructed using the fitness values  $f(x_1^{(g)}), \dots, f(x_\lambda^{(g)})$  of individuals from some particular generation or several generations of CMA-ES. Its construction can be as simple as setting  $\bar{f}$  to a constant aggregating the considered fitness values, e.g., their mean or weighted mean, but it can also consist in training, with those values, a response surface model, principally of any kind.
2. Kruisselbrink et al. [16], who combine CMA-ES with a GP using the  $\gamma$ -exponential function  $K$ , propose to employ in (15) the Mahalanobis distance of vectors  $x$  and  $x'$  given by the covariance matrix obtained in the  $g$ -th generation of CMA-ES,  $(\sigma^{(g)})^2 C^{(g)}$ , instead of their Euclidean distance. This is actually a specific consequence of another possibility of using information from CMA-ES for the GP – replacing the original space of  $d$ -dimensional vectors,  $\mathbb{R}^d$ , by the space of their principal components with respect to  $C^{(g)}$ . In this context, it is worth recalling that in [2, 3, 15], Mahalanobis instead of Euclidean distance was used when combining CMA-ES with quadratic response surface models in [2, 3, 15]. In the approach presented there, the space of the principal components with respect to  $C^{(g)}$  is used, together with an estimate of density, to locally weight the model predictions with respect to the considered input. In this way, a connection to the other kind of synergy is established, i.e., to the evolution control of CMA-ES, giving us the possibility to use both kinds in combination.

#### 3.2 GP-Based Evolution Control of CMA-ES

We intend to test the following approaches to using GP for the evolution control of CMA-ES.

- (i) *Basic approach.* In the  $(g+1)$ -th generation,  $\lambda'$  points  $\tilde{x}_1, \dots, \tilde{x}_{\lambda'} \in \mathbb{R}^d$  are sampled from the distribution  $N(m^{(g)}, (\sigma^{(g)})^2 C^{(g)})$ , where  $\lambda'$  is several to many times larger than  $\lambda$ . For all of them, a selected criterion from among those introduced in 2.1

### Algorithm 1

Input: generation  $g$ , points  $\tilde{x}_1, \dots, \tilde{x}_{\lambda'} \in \mathbb{R}^d \sim N(m^{(g)}, (\sigma^{(g)})^2 C^{(g)})$ , their linear ordering  $\prec_c, c \in \{Q_\alpha, \text{PoI}, \text{EI}\}$  with  $\alpha \in (0, 1)$  according to a GP-based criterion to choose the points for evaluation,  $\lambda \in \mathbb{N}, \lambda < \text{card}\{\tilde{x}_1, \dots, \tilde{x}_{\lambda'}\}, k \in \{1, \dots, \lambda\}$ .

Step 1. Perform  $k$ -means clustering of  $S = \{\tilde{x}_1, \dots, \tilde{x}_{\lambda'}\}, k \in \{1, \dots, \lambda\}$  into sets  $S_1, \dots, S_k$ .

Step 2. For  $j = 1, \dots, k$ , choose  $x_j^{(g+1)} = \max_{\prec_c} S_j$ .

Step 3. For  $j = k + 1, \dots, \lambda$ , choose  $x_j^{(g+1)} = \max_{\prec_c} S \setminus \{x_i^{(g+1)} : i = 1, j - 1\}$ .

Output: Points  $x_1^{(g+1)}, \dots, x_\lambda^{(g+1)}$  to be evaluated by the original fitness function.

Figure 1: Algorithm of the proposed strategy for choosing the  $\lambda$  points to be evaluated by the original fitness from among the  $\lambda'$  evaluated by the Gaussian process

is computed. Based on the value of that criterion, the  $\lambda$  points  $x_1^{(g+1)}, \dots, x_\lambda^{(g+1)}$  for the evaluation by the original black-box fitness are chosen. This can be done according to various strategies, we intend to use the one described in Algorithm 1, with which we have a good experience from using radial basis function networks for the evolution control in the evolutionary optimization of catalytic materials [10]. The linear ordering  $\prec_c$  stands in the cases  $c = \text{PoI}$  and  $c = \text{EI}$  for  $\leq$ , in the case  $c = Q_\alpha$  for  $\geq$ . The use of a linear ordering relates the proposed approach to ranking-based evolution control of CMA-ES [2, 3, 15, 23], as well as to surrogate modelling of CMA-ES by ordinal regression [17, 18, 19, 22]. Most similar is the approach by Ulmer et al. [23], the difference being that they don't use clustering.

- (ii) *GP on low-dimensional projections* attempts to improve the basic approach in view of the experience reported in the literature [15] and obtained also in our earlier experiments [1] that GPs are actually advantageous only in low dimensional spaces. Instead of the sampled points  $\tilde{x}_1, \dots, \tilde{x}_{\lambda'}$ , the GP is trained only with their first  $\ell < d$  principal components with respect to  $C^{(g)}$ ,  $\tilde{x}_1^{[\ell]}, \dots, \tilde{x}_{\lambda'}^{[\ell]}$ , i.e., with the projections of  $\tilde{x}_1, \dots, \tilde{x}_{\lambda'}$  to the  $\ell$ -dimensional space  $\mathbb{X}_\ell = \text{span}(b_1^{(g)}, \dots, b_\ell^{(g)})$ , provided the orthonormal eigenvectors  $b_i^{(g)}$  are enumerated according to decreasing eigenvalues.
- (iii) *GP on low-dimensional projections within restricted distance* attempts to decrease the deterioration of the GP on low-dimensional projections with respect to the GP on the original sampled points  $\tilde{x}_1, \dots, \tilde{x}_{\lambda'}$  by using only points  $\tilde{x}_i$  within a prescribed small distance  $\epsilon$  from their respective projections  $\tilde{x}_i^{[\ell]}$ . To this end, points from the distribution  $N(m^{(g)}, (\sigma^{(g)})^2 C^{(g)})$  are resampled until  $\lambda'$  points  $\tilde{x}_i$  are obtained fulfilling

$$\|\tilde{x}_i - \tilde{x}_1^{[\ell]}\| < \epsilon, \text{ or equivalently, } \|\tilde{x}_i\|^2 - \|\tilde{x}_1^{[\ell]}\|^2 < \epsilon^2. \quad (25)$$

- (iv) *Two-stage sampling.* Training the GP for the  $(g + 1)$ -th generation can easily suffer from the lack of training data in a part of the search space where a substantial proportion of the points  $\tilde{x}_1, \dots, \tilde{x}_{\lambda'}$  will be sampled. To alleviate it, the points  $x_1^{(g+1)}, \dots, x_\lambda^{(g+1)}$  to be evaluated by the original fitness can be sampled in two stages:

1. First, points  $x_1^{(g+1)}, \dots, x_{\lambda''}^{(g+1)}$ , where  $\lambda'' < \lambda$ , are sampled from the distribution  $N(m^{(g)}, (\sigma^{(g)})^2 C^{(g)})$ , evaluated by the original fitness, and included into training the GP.

2. Then,  $\lambda'$  points  $\tilde{x}_1, \dots, \tilde{x}_{\lambda'}$  are sampled from the same distribution, and for them, a selected criterion from among those introduced in 2.1 is computed, based on which the points  $x_{\lambda''+1}^{(g+1)}, \dots, x_{\lambda}^{(g+1)}$  for the evaluation by the original black-box fitness are chosen. To this end, again Algorithm 1 can be used, with the following changes:

- In the input, the numbers  $\lambda'$  and  $k$  have now to fulfill

$$\lambda - \lambda'' < \text{card}\{\tilde{x}_1, \dots, \tilde{x}_{\lambda'}\}, k \in \{1, \dots, \lambda - \lambda''\}. \quad (26)$$

- In Step 3,  $x_j^{(g+1)} = \max_{\prec_c} S \setminus \{x_i^{(g+1)} : i = 1, j - 1\}$  is chosen only for  $j = k + 1, \dots, \lambda - \lambda''$ .
- The output contains only the points  $x_{\lambda''+1}^{(g+1)}, \dots, x_{\lambda}^{(g+1)}$ .

Needless to say, this approach has to be combined with some of the approaches (i)–(iii) and can be combined with any of them.

- (v) *Generation-based evolution control.* Whereas the previous four approaches represent, in terms of [11, 12], individual-based evolution control, we want to test also one approach that is generation-based, in the sense that the desired number  $\lambda$  of points is evaluated by the original black-box fitness function only in selected generations. Similarly to the evolution strategy in [18, 19], our approach selects those generations adaptively, according to the agreement between the ranking of considered points by the surrogate model and by the black-box fitness. Differently to that strategy, however, we want to base the estimation if that agreement not on the generations in which  $\lambda$  points have been evaluated by the black-box fitness, but on evaluating a small and evolvable number  $\lambda'''$  of additional points in each generation. In this context, it is important that in situations when the fitness is evaluated empirically, using some measurement or testing, the evaluation hardware causes the evaluation costs to increase step-wise, and to remain subsequently constant for some  $\lambda_{\text{hw}}$  evaluated points (e.g. in the optimization of catalyst preformance described in [10],  $\lambda_{\text{hw}}$  is the number of channels in the chemical reactor in which the catalysts are tested). In such a situation, the costs of evaluation are the lowest if  $\lambda$  is a multiple of  $\lambda_{\text{hw}}$ , and if the evaluation of the  $\lambda'''$  additional points in each generation is cumulated for  $n_{\text{hw}}$  generations such that

$$n_{\text{hw}} = \max_{n \in \mathbf{N}} n\lambda''' \leq \lambda_{\text{hw}}. \quad (27)$$

Setting  $n_{\text{hw}} = 1$  covers the case when such a situation does not occur and the evaluation costs increase linearly with the number of points. If  $g_{\text{last}}$  is the last generation in which  $\lambda$  points have been evaluated by the black-box fitness, then for  $g = g_{\text{last}}, \dots, g_{\text{last}} + n_{\text{hw}} - 1$ , points  $\tilde{x}_1^{g+1}, \dots, \tilde{x}_{\lambda'}^{g+1} \in \mathbb{R}^d$  are sampled from the distribution  $N(m^{(g)}, (\sigma^{(g)})^2 C^{(g)})$ , from which the points  $x_1^{(g+1)}, \dots, x_{\lambda'''}^{(g+1)}$  are selected by Algorithm 1, in which the input  $\lambda$  is replaced with  $\lambda'''$ . Subsequently, all the points  $x_1^{(g_{\text{last}}+1)}, \dots, x_{\lambda'''}^{(g_{\text{last}}+n_{\text{hw}})}$  are evaluated by the black-box fitness, and for each generation  $g = g_{\text{last}} + 1, \dots, g_{\text{last}} + n_{\text{hw}}$ , the agreement between the ranking of  $x_1^g, \dots, x_{\lambda'''}^g$  by the current Gaussian process,  $\text{GP}_{\text{current}}$ , and the black-box fitness is estimated. If the agreement is sufficient in all considered generations, then the procedure is repeated using  $g_{\text{last}} + n_{\text{hw}}$  instead of  $g_{\text{last}}$  and unchanged  $\lambda'''$ . Otherwise, additional

points  $x_{\lambda''' + 1}^g, \dots, x_{\lambda''' + \lambda}^g$  are selected from  $\tilde{x}_1^g, \dots, \tilde{x}_{\lambda'}^g$  for the first generation  $g$  in which the agreement was not sufficient. Then a new Gaussian process,  $\text{GP}_{\text{new}}$ , is trained using the training set

$$T_{\text{new}} = \bigcup_{g'=1}^g \{x_1^{g'}, \dots, x_{\lambda'''}^{g'}\} \cup \{x_{\lambda''' + 1}^g, \dots, x_{\lambda''' + \lambda}^g\}, \quad (28)$$

optionally including also some or all points from the set  $T_{\text{current}}$  used for training  $\text{GP}_{\text{current}}$ . At that occasion, also the value of  $\lambda'''$  can be changed.

Provided the conditions  $1 \leq \lambda''' < \lambda$  and  $\lambda''' + \lambda \leq \lambda'$  are fulfilled, the value of  $\lambda'''$  can be arbitrary. Needless to say, the smaller  $\lambda'''$ , the larger will be the proportion of points from the generation in which the GP was trained in its training set, and the more similar the obtained GP will normally be to a GP trained only with data from that generation, which is the usual way of using surrogate models in traditional generation-based strategies [11, 12, 18, 19]. It is also worth pointing out that our generation-based evolution control was explained here as a counterpart to the basic individual-based approach (i), but counterparts to the approaches (ii) and (iii) are possible as well.

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